



Improvements to the CAMx Photochemical Model for Winter Ozone

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Air Quality in Utah: Science for Solutions II

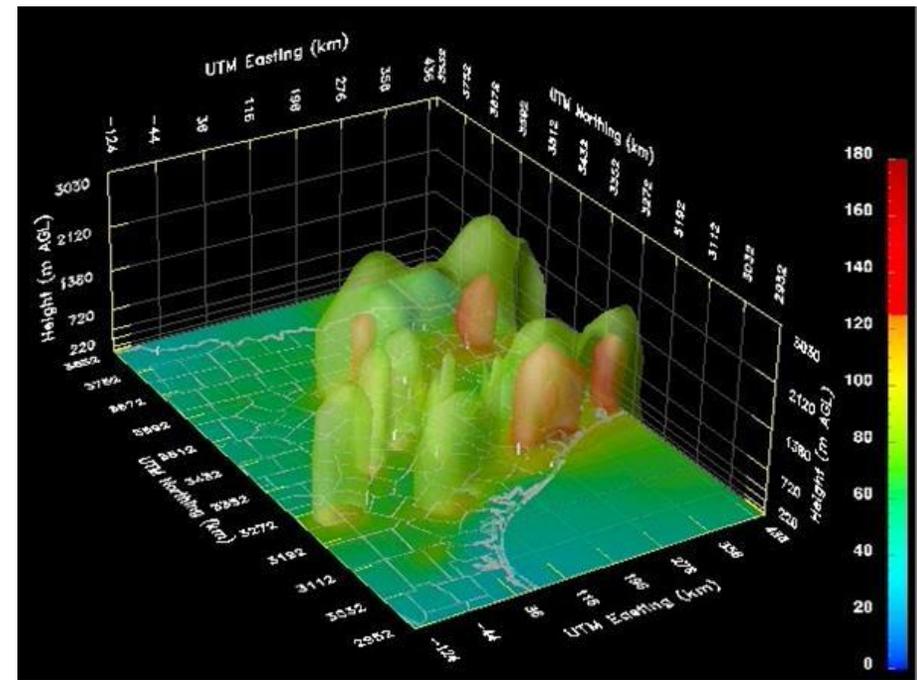
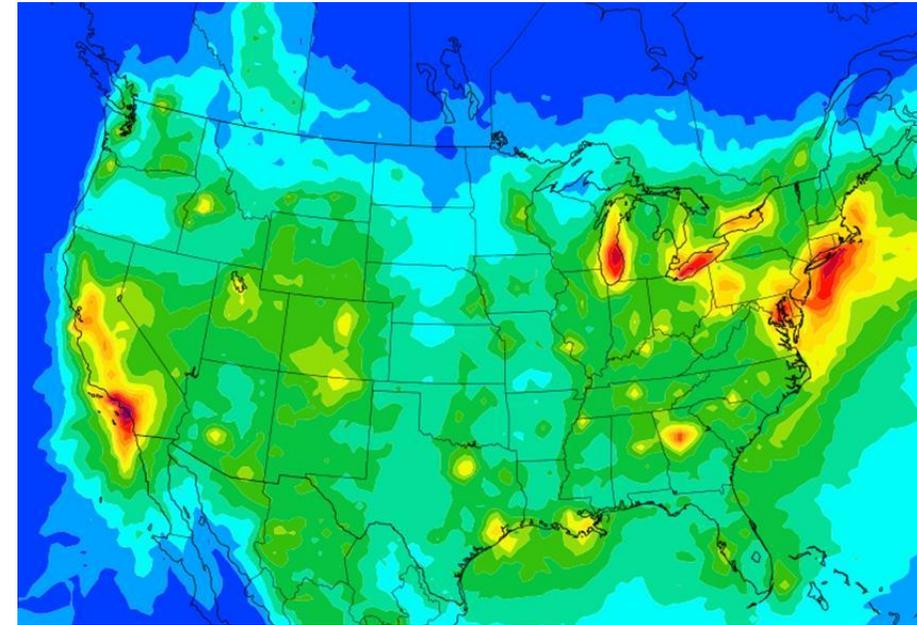
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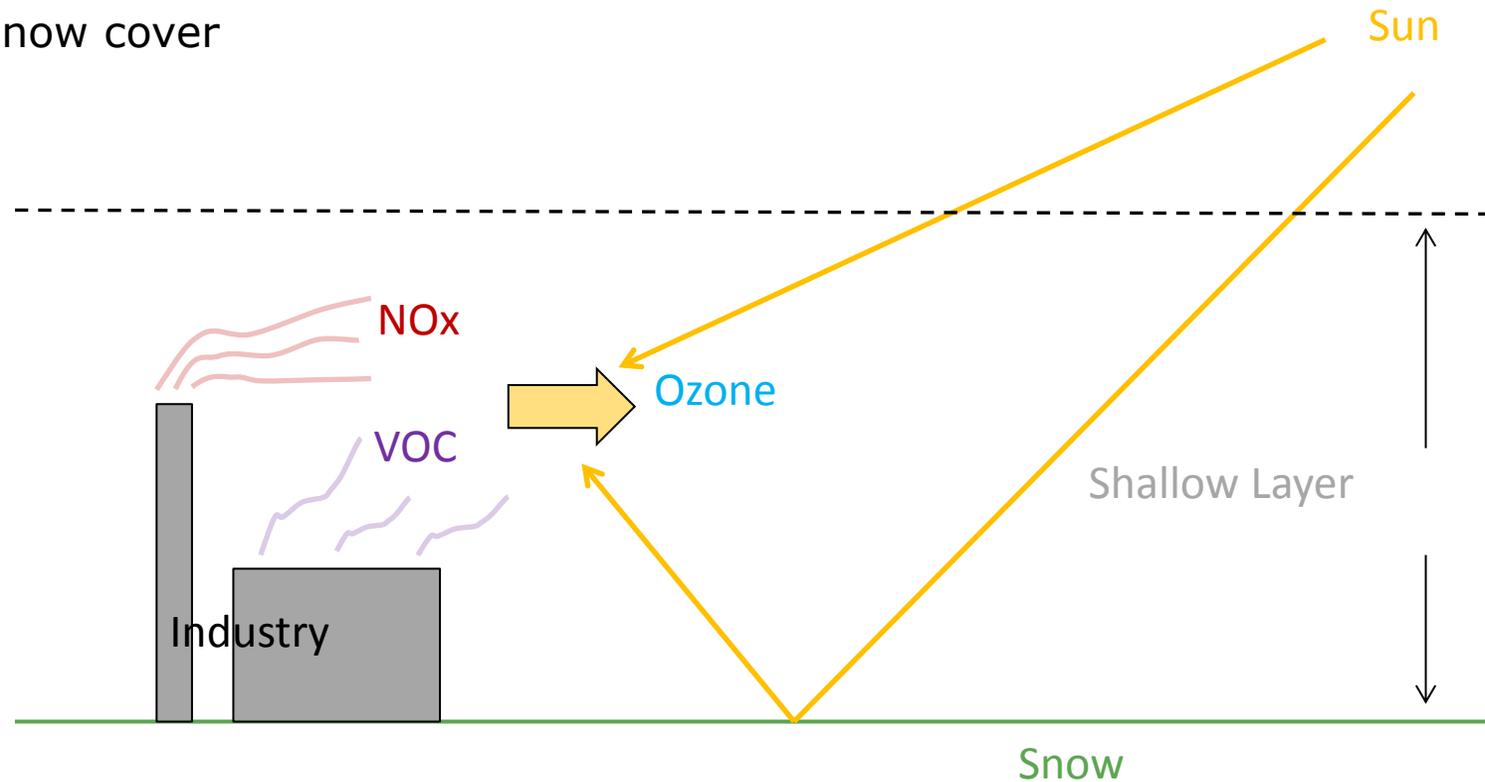
WHAT IS CAMx?

- A three-dimensional photochemical grid model
 - It's like a weather prediction model, BUT:
 - It simulates the movement and chemical evolution of pollutants through the atmosphere
- Such models help us:
 - Explain observed conditions
 - Understand complex processes
 - Identify source culpability
 - Investigate mitigation strategies
- CAMx needs many types of "big" data
 - Emissions, meteorology, surface characteristics, etc.



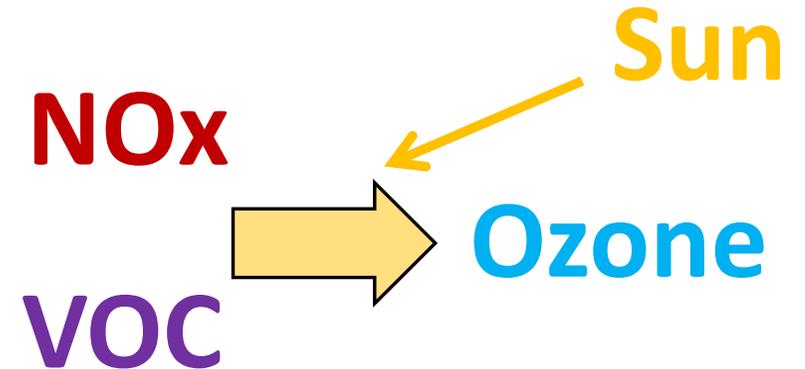
PROJECT PURPOSE

- This project looks to improve on two pieces of the difficult wintertime ozone modeling puzzle
 - 1) Atmospheric chemistry for western Oil & Gas basin conditions
 - 2) Treatment of snow cover

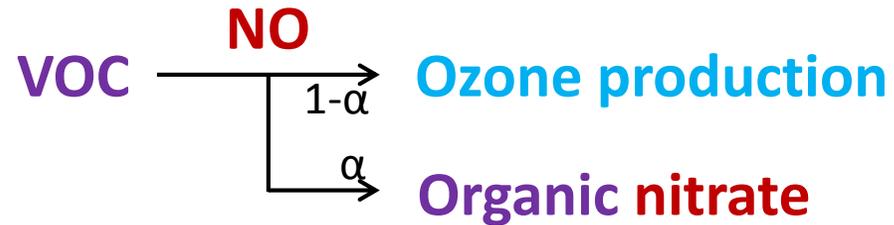


ARE CHEMISTRY CHANGES NEEDED FOR WINTER OZONE?

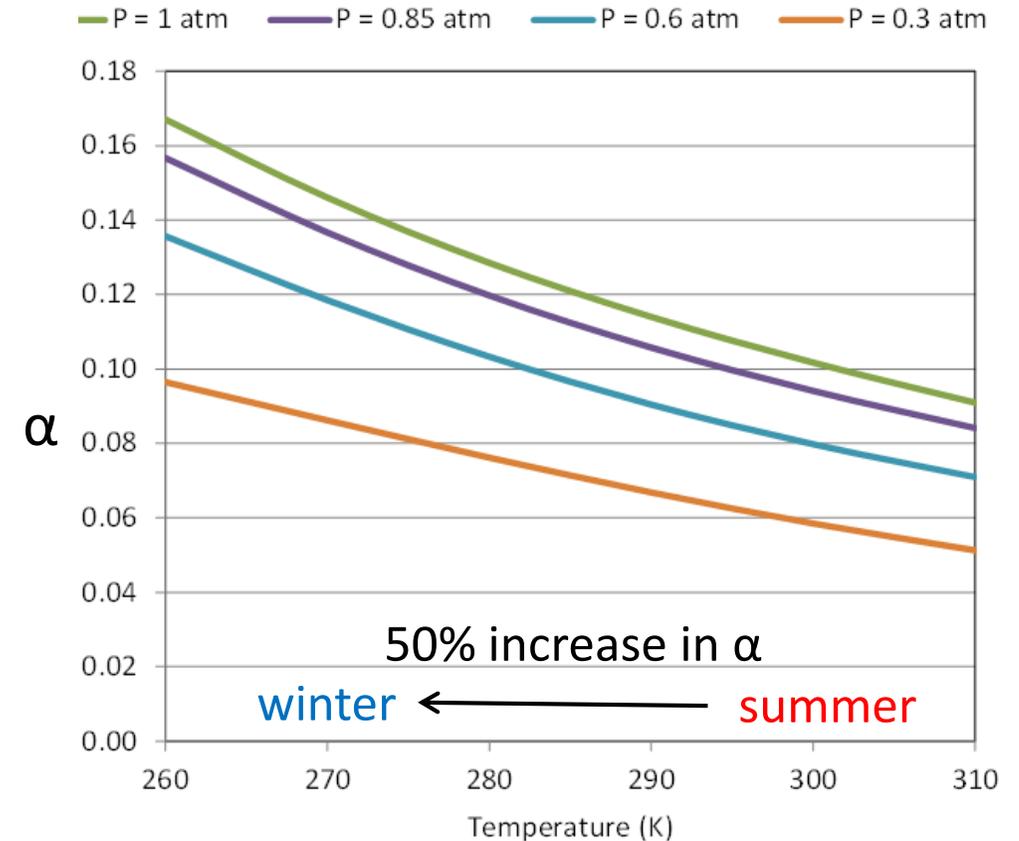
- Photolytic effect of **sunlight**
 - Little variation with temperature
- Chemistry of **NO_x** and similar molecules
 - Cold conditions are understood
 - NO_x chemistry is important for ozone from surface through stratosphere
- Chemistry of **VOC**
 - Models developed for summer ozone
 - There is potential for improvement
 - Focus on the most abundant VOCs in western US O&G basins: **Alkanes**



ALKANE CHEMISTRY



- Fraction (α) of **organic nitrate** formed depends on temperature and pressure (altitude)
 - But models hold α constant
 - Including this dependency should improve winter chemistry modeling
 - Important for O&G basin conditions
- Dynamic branching ratio added to CB6(r3)



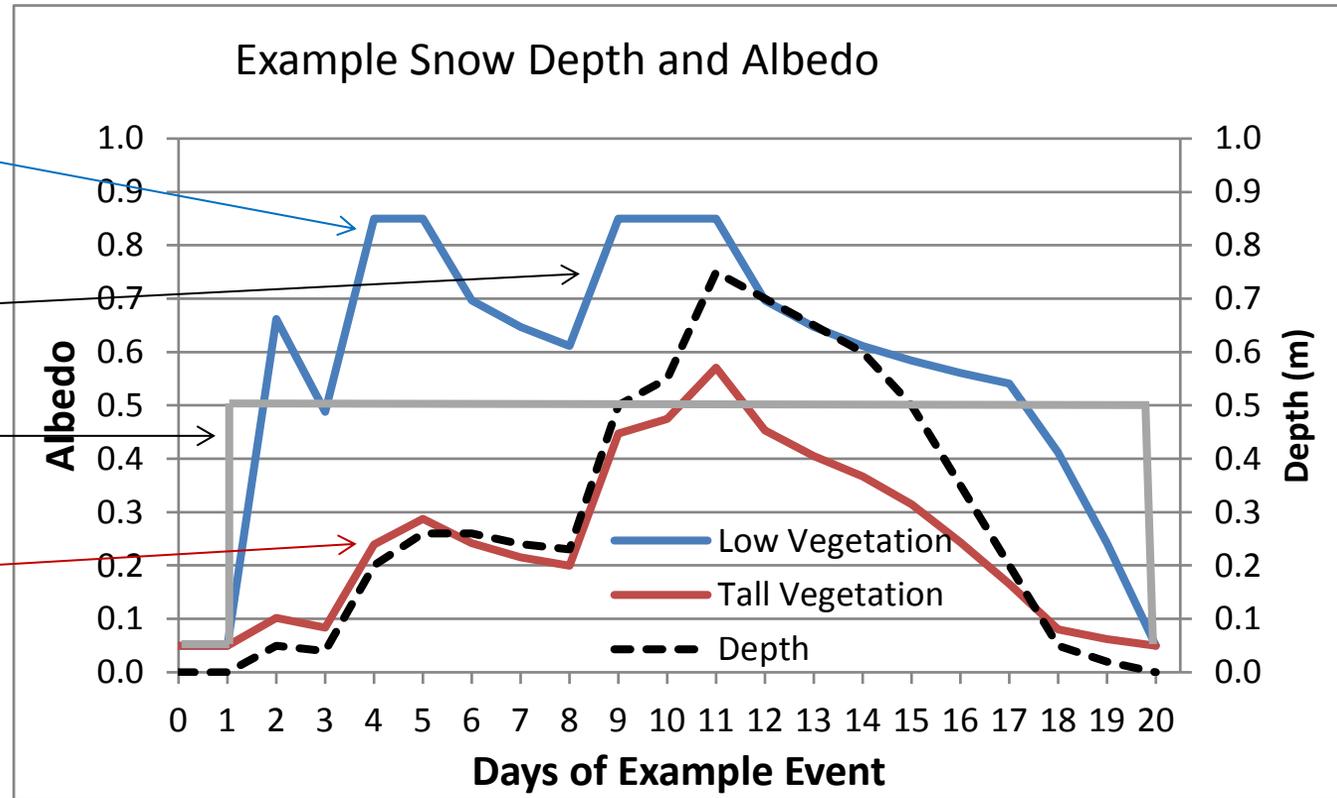
IMPROVEMENTS FOR SNOW ALBEDO

Low vegetation covered faster/completely, maximizing snow albedo

New snowfall increases snow depth and “freshens” the albedo

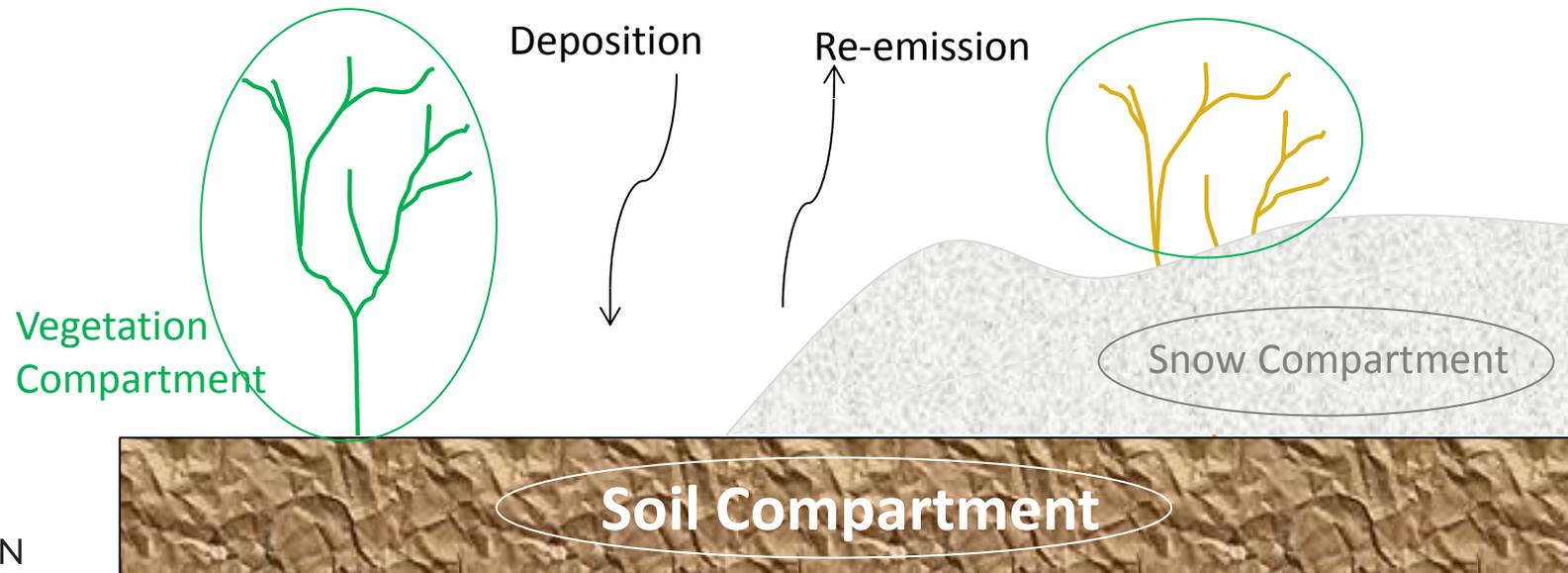
Original albedo assumption

Tall vegetation covered slower/incompletely, minimizing snow albedo



SURFACE CHEMISTRY UPDATE

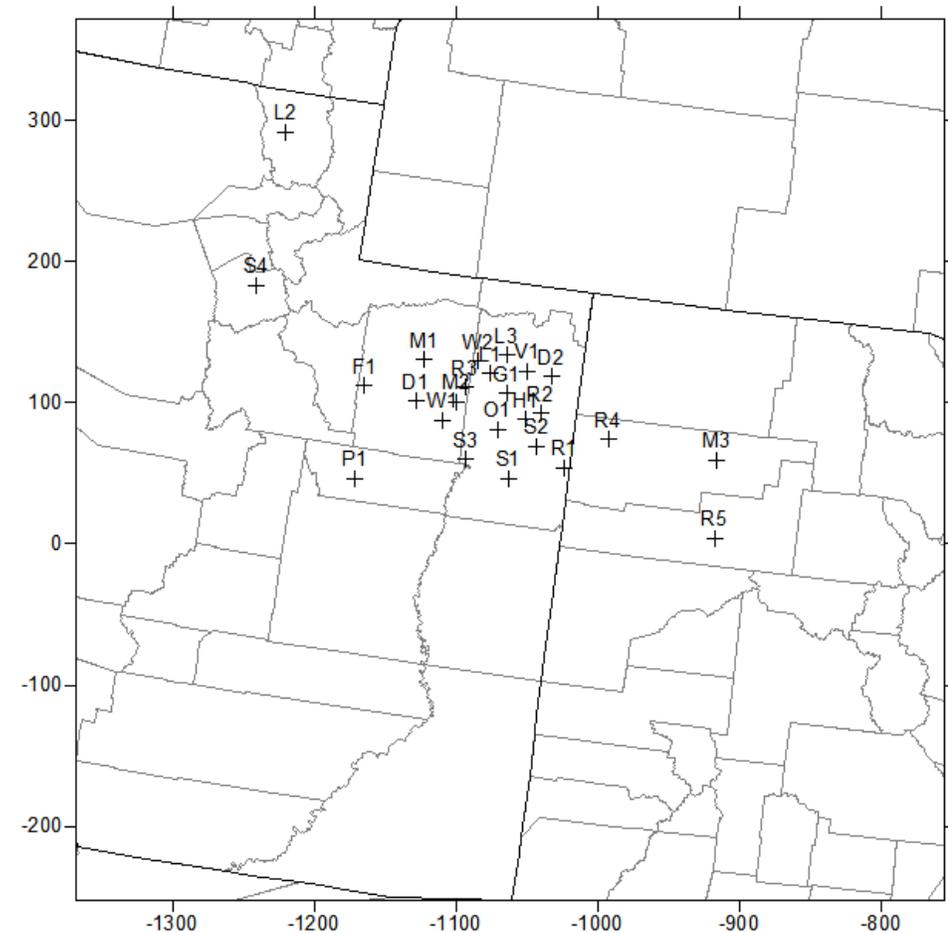
- Optional model component:
 - Two-way transfer between atmosphere and surface system
 - Chemical interactions among deposited material form products that re-emit
- Updated to include snow with soil and vegetation compartments
- Do models need to account for snow surface-atmosphere chemistry interaction?
 - May be an important contributor to atmospheric chemistry



EVALUATION IN UINTA BASIN

- **Model:**
 - CAMx v6.1 with snow/chemistry updates
- **Domain:**
 - UDAQ 4-km grid over eastern Utah
 - February 1-7, 2013 (during UBOS)
- **Datasets:**
 - UofU-derived meteorology
 - (Initial) Older UDAQ-derived emissions
 - (Latest) NEIv2/UDAQ-derived emissions
 - Boundary conditions from a global model
 - NOAA/UBOS 2013 measurements

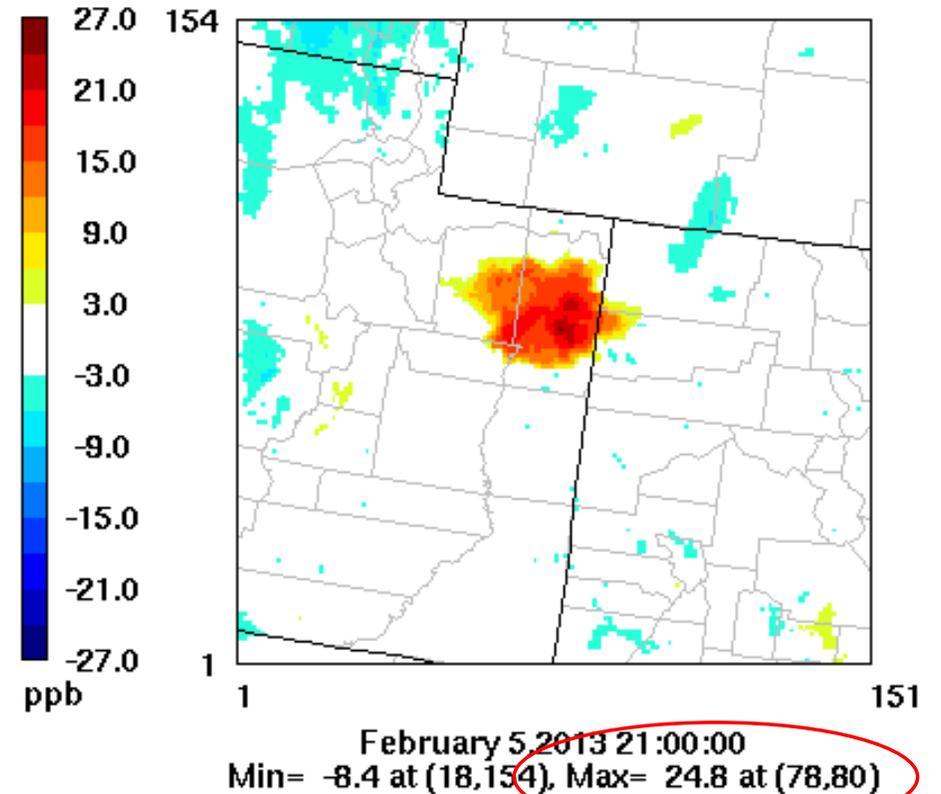
O3 observation sites in the UDAQ 4km



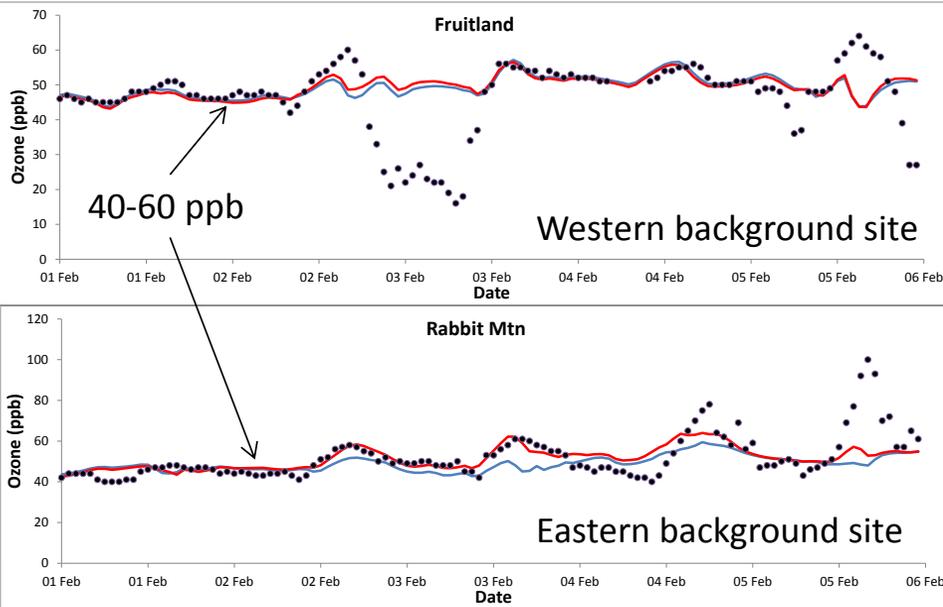
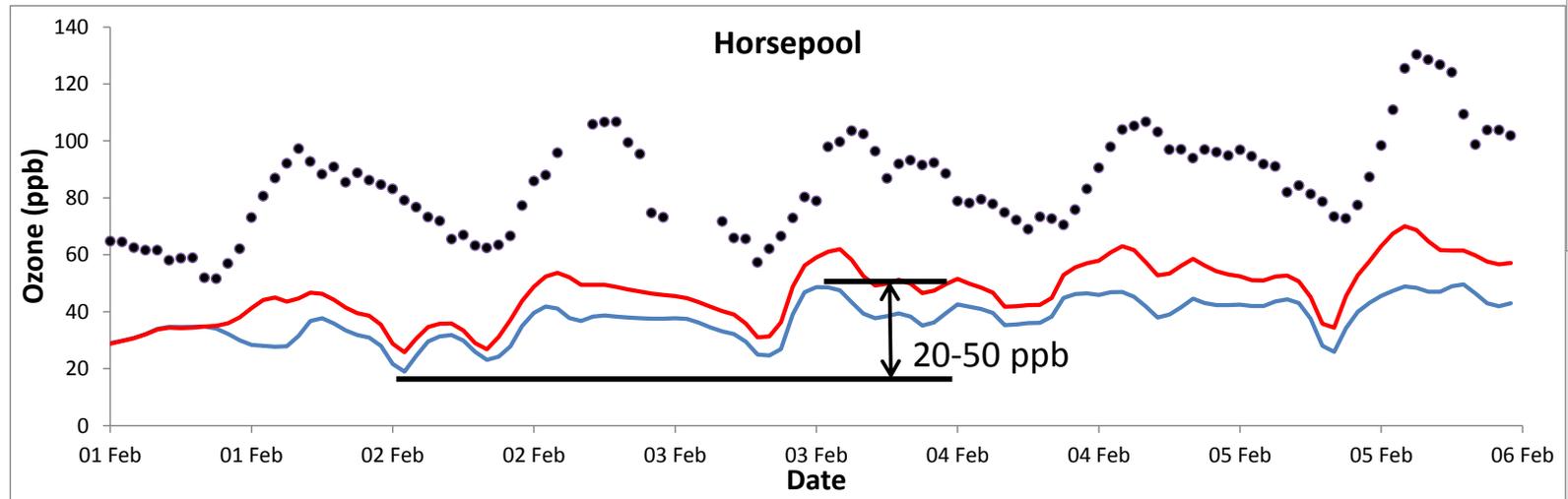
INITIAL OZONE SIMULATIONS

- Total effect of all model updates:
 - 10-20 ppb O₃ **increase**
- Snow albedo/deposition update:
 - O₃ **increase**
- Winter chemistry update:
 - O₃ **decrease**
- Surface chemistry update re-emitting HONO:
 - O₃ **increase**
 - Surface chemistry configured for **testing purposes only!**
 - Highly speculative, currently no conclusive evidence for a surface chemical pathway

Effect with New Snow + Chemistry Update + Surface Model w/ Snow



INITIAL OZONE SIMULATIONS

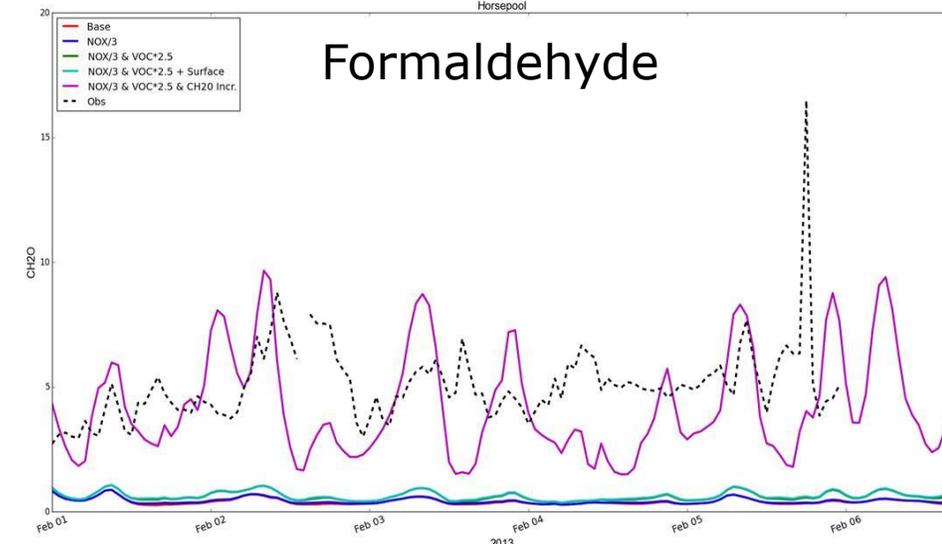
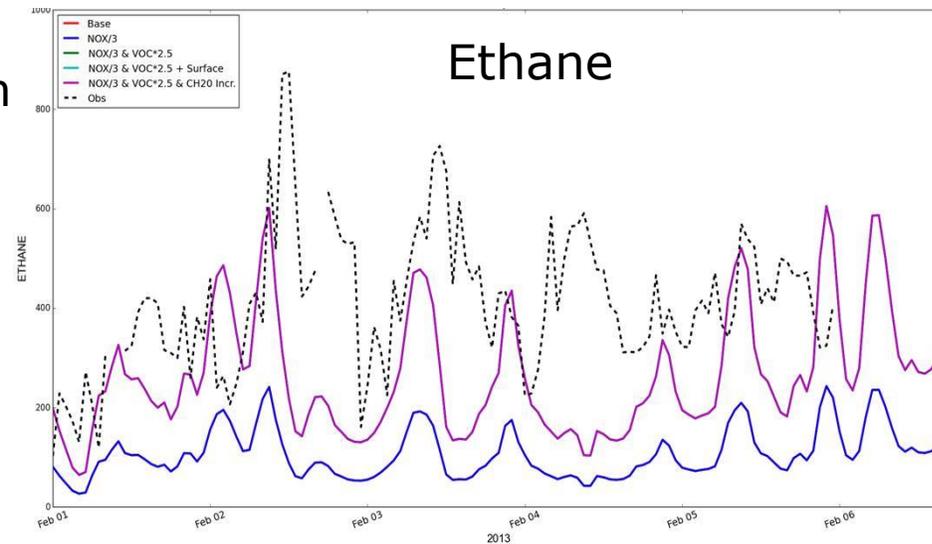
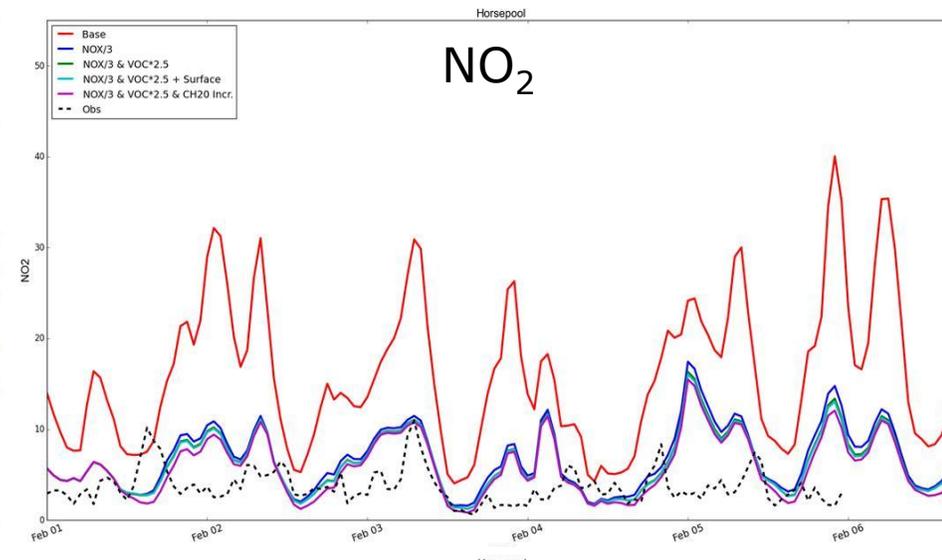
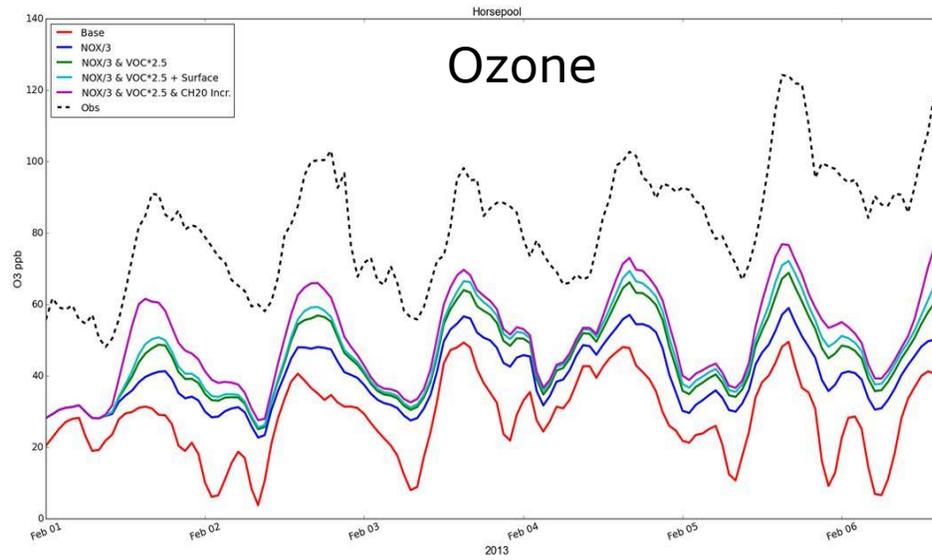


— Original Model
— New snow + Chemistry Update + Surface Model w/ Snow

- O_3 is too low in the basin
 - O_3 is inhibited and suppressed
 - Comparisons to 2013 UBOS measurements confirm model is NO_x -rich, VOC-poor
- But background is higher and better simulated outside the basin

LATEST OZONE SIMULATIONS

- Base (CB6r3+snow)
- NO_x/3
- NO_x/3+VOC×2.5
- NO_x/3+VOC×2.5+Surface Model
- NO_x/3+VOC×2.5+Formaldehyde
- Still not getting enough ozone
- Ratios of N compounds are wrong – implies missing reactivity



SUMMARY

- CAMx improvements lead to positive effects, in line with expectations
 - Air chemistry: cold temperatures push NO_x out of ozone cycle, reduces ozone slightly
 - Snow: higher albedo, reductions in deposition increase ozone
 - Surface/snow chemistry:
 - May be a source of emissions that increase reactivity and ozone production
 - Complex, uncertain, inconclusive – more study needed, but CAMx now has this capability
 - These updates are insufficient to simulate ozone at measured levels
- Need additional work on emission estimates
 - NO_x oxidation products are not correctly replicated: emission-chemistry cycle is not right
 - Too much NO_x: over estimated inventory or improper vertical distribution?
 - Too little VOC: under estimating fugitive emissions?
 - Too little formaldehyde: missing a source, ubiquitous use of methanol?

**THANK YOU
QUESTIONS?**